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Geometrical Stabilities and Electronic Structures of Rh5 Nanoclusters on Rutile TiO₂ (110) for Green Hydrogen Production

Abstract:

Addressing the urgent need for sustainable energy sources, this study investigates the intricate relationship between Rhodium (Rh5) nanoclusters and TiO₂ rutile (110) surfaces, aiming to advance photocatalytic water splitting for green hydrogen production. Motivated by the imperative to transition from conventional fossil fuels, the study employs density functional theory (DFT) with DFT-D3 and HSE06 hybrid functional to analyse the geometrical stabilities and electronic structures of Rh5 nanoclusters on TiO₂ rutile (110). TiO₂, a prominent photocatalyst, faces challenges such as limited visible light absorption, leading researchers to explore noble metals like Rh as cocatalysts. Our results show that bipyramidal Rh5 nanoclusters exhibit enhanced stability and charge transfer when adsorbed on TiO₂ rutile (110) compared to trapezoidal configurations. The most stable adsorption induces oxidation of the nanocluster, altering the electronic structure of TiO₂. Extending the analysis to defective TiO₂ surfaces, the study explores the impact of Rh5 nanoclusters on oxygen vacancy formation, revealing stabilisation of TiO₂ and increased oxygen vacancy formation energy. This theoretical exploration contributes insights into the potential of Rh5 nanoclusters as efficient cocatalysts for TiO₂-based photocatalytic systems, laying the foundation for experimental validations and the rational design of highly efficient photocatalysts for sustainable hydrogen production. The observed effects on electronic structures and oxygen vacancy formation emphasize the complex interactions between Rh5 nanoclusters and TiO₂ surface, guiding future research in the quest for clean energy alternatives.

Biography

Moteb Qahess Mansour Alotaibi is an Assistant Professor in the Department of Physics at the College of Science and Humanity Studies in Alkharj. He holds a PhD in Nanoscience from Lancaster University (2023), an MSc in Condensed Matter Physics from Ottawa University (2019), and a BSc in Physics from Prince Sattam bin Abdulaziz University (2013). His research interests include hydrogen energy production, quantum transport in molecules, photocatalysis, and thermal barrier coatings. Dr. Alotaibi has been an active member of the Student Accommodation Committee since 2013 and coordinates conventions, external partnerships, and social responsibility initiatives within the Physics department. Additionally, he serves as the Chair of the Academic Committee, demonstrating his dedication to academic excellence and community engagement.